



# Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2021 – 10:11 pm BST

PDB ID : 2WG0  
Title : AGED CONJUGATE OF TORPEDO CALIFORNICA ACETYL-  
CHOLINESTERASE WITH SOMAN (OBTAINED BY IN CRYSTALLO  
AGING)  
Authors : Sanson, B.; Nachon, F.; Colletier, J.P.; Froment, M.T.; Toker, L.; Greenblatt,  
H.M.; Sussman, J.L.; Ashani, Y.; Masson, P.; Silman, I.; Weik, M.  
Deposited on : 2009-04-15  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

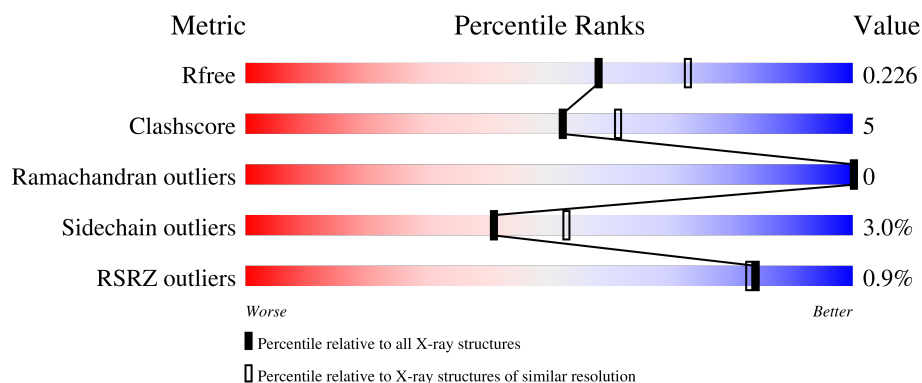
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


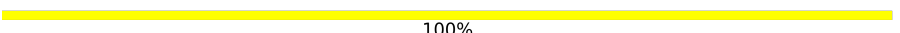
The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	537	 88% 10% ..
2	B	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	2536	-	-	-	X
9	PEG	A	2551	-	-	X	-
9	PEG	A	2555	-	-	X	-

## 2 Entry composition [i](#)

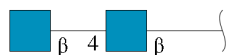
There are 10 unique types of molecules in this entry. The entry contains 5113 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

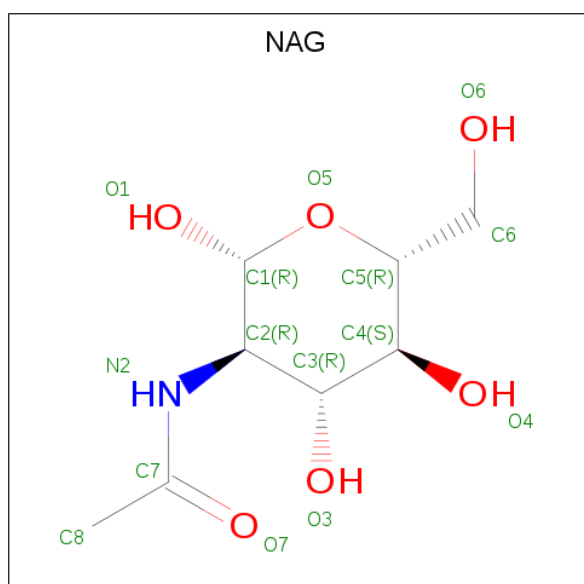
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4297	2760	728	785	24	0	9	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

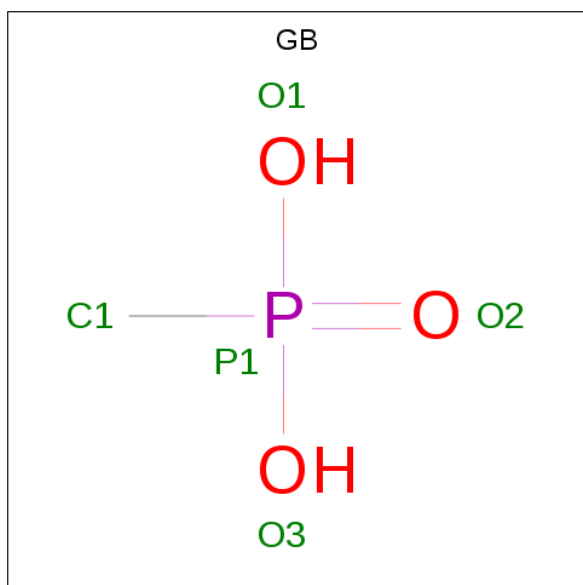


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

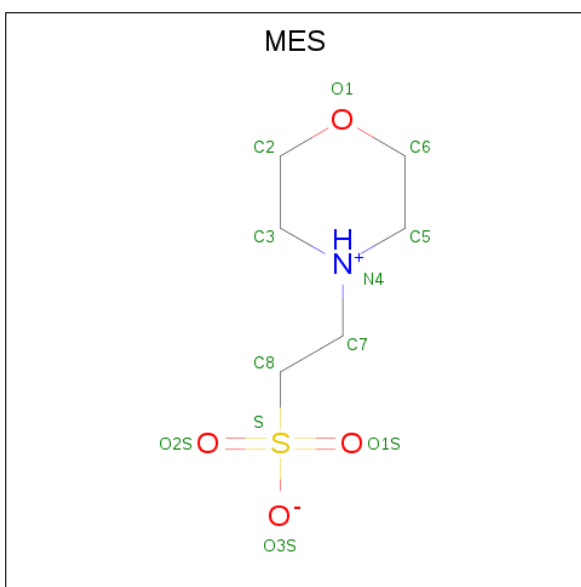
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is METHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: GB) (formula: CH<sub>5</sub>O<sub>3</sub>P).



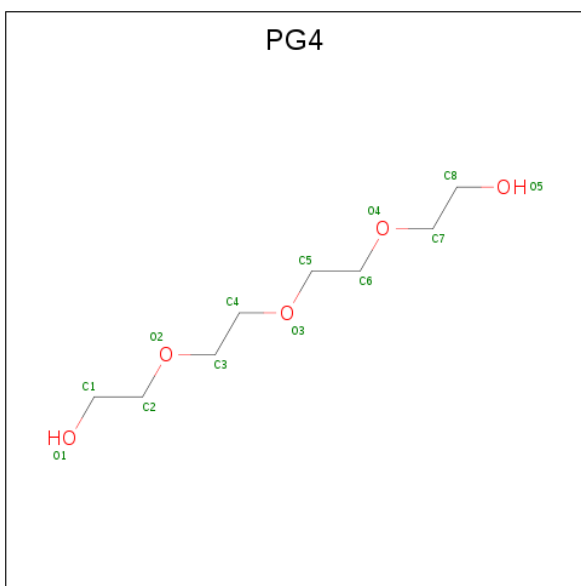
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			4	1	2	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



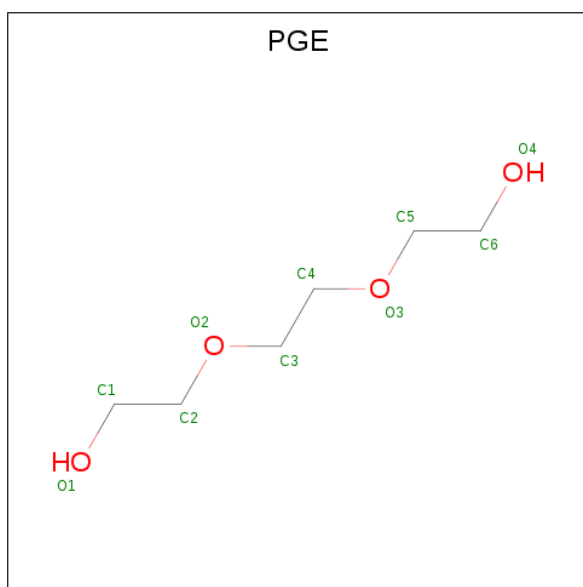
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



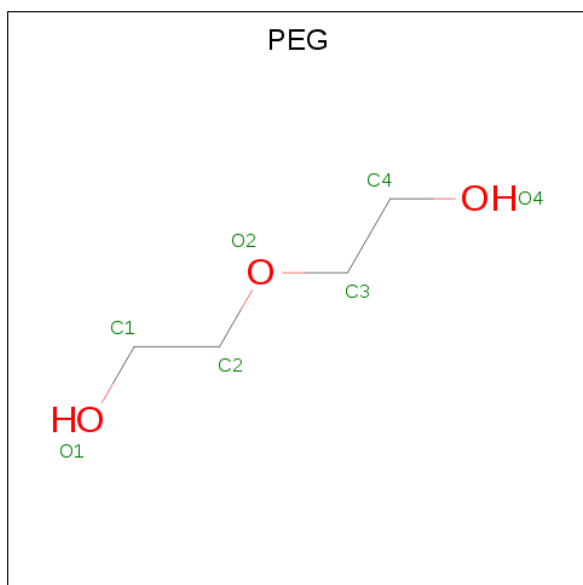
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0

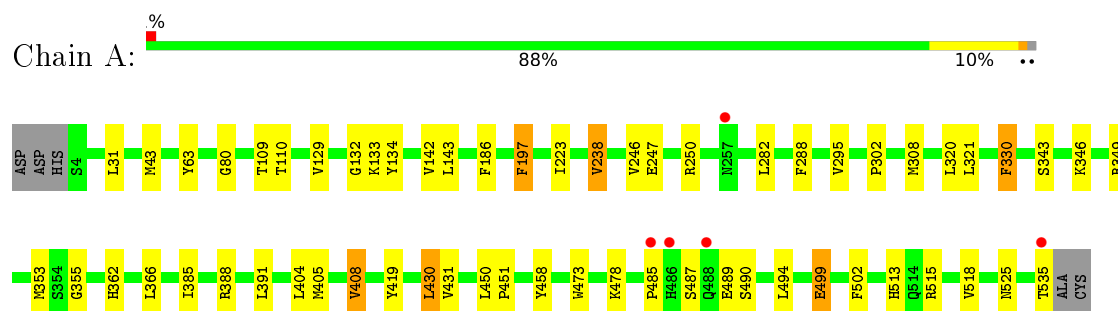
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	620	Total O 620 620	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ACETYLCHOLINESTERASE



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.61Å 111.61Å 136.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 2.20 48.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.34-2.20) 99.4 (48.33-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.177 , 0.229 0.177 , 0.226	Depositor DCC
$R_{free}$ test set	2459 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, CL, MES, PG4, PEG, GB, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.69	0/4447	0.69	1/6031 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	388	ARG	NE-CZ-NH2	-6.86	116.87	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4297	0	4184	45	0
2	B	28	0	25	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	4	0	3	0	0
6	A	12	0	13	1	0
7	A	13	0	18	0	0
8	A	40	0	56	2	0
9	A	70	0	100	15	0
10	A	620	0	0	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5113	0	4425	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353[B]:MET:CE	10:A:1176:HOH:O	1.97	1.13
1:A:431:VAL:HG22	9:A:2555:PEG:H42	1.47	0.97
1:A:353[B]:MET:SD	10:A:1176:HOH:O	2.24	0.95
1:A:478[A]:LYS:HE3	10:A:1186:HOH:O	1.71	0.91
1:A:525:ASN:HD22	9:A:2551:PEG:H12	1.36	0.89
1:A:80:GLY:HA2	9:A:2555:PEG:H32	1.65	0.78
1:A:353[B]:MET:HE3	10:A:1176:HOH:O	1.71	0.76
9:A:2549:PEG:H32	10:A:1613:HOH:O	1.89	0.72
1:A:321:LEU:HD11	1:A:408:VAL:HG12	1.73	0.70
9:A:2551:PEG:H11	10:A:1575:HOH:O	1.91	0.70
1:A:525:ASN:ND2	9:A:2551:PEG:H12	2.07	0.70
1:A:404:LEU:O	1:A:408:VAL:HG13	1.95	0.67
1:A:430:LEU:HD23	9:A:2555:PEG:H41	1.76	0.67
1:A:353[B]:MET:CG	10:A:1176:HOH:O	2.46	0.64
1:A:431:VAL:H	9:A:2555:PEG:H42	1.64	0.63
1:A:499:GLU:HG3	10:A:1537:HOH:O	2.00	0.62
1:A:246:VAL:HG22	9:A:2548:PEG:H11	1.83	0.60
1:A:43:MET:HE3	10:A:1049:HOH:O	2.00	0.60
1:A:349:ARG:O	1:A:353[A]:MET:HG2	2.06	0.56
1:A:405:MET:HB3	9:A:2551:PEG:H42	1.88	0.54
1:A:485:PRO:HA	10:A:1523:HOH:O	2.08	0.53
1:A:478[A]:LYS:HD2	10:A:1512:HOH:O	2.08	0.53
1:A:302:PRO:HD2	1:A:308:MET:SD	2.49	0.52
1:A:353[B]:MET:HG2	10:A:1176:HOH:O	2.09	0.52
1:A:109:THR:CG2	1:A:142:VAL:HG23	2.40	0.51
1:A:223:ILE:HA	1:A:320:LEU:O	2.11	0.50
1:A:431:VAL:H	9:A:2555:PEG:C4	2.25	0.50
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.48	0.49
8:A:2544:PGE:H12	9:A:2550:PEG:H32	1.95	0.49
1:A:197:PHE:CB	1:A:223:ILE:HB	2.43	0.49
1:A:362:HIS:HA	10:A:1405:HOH:O	2.11	0.49
1:A:346:LYS:HG2	1:A:385:ILE:HD13	1.95	0.48
1:A:238:VAL:HG23	1:A:295:VAL:HG22	1.96	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:N	1:A:451:PRO:CD	2.77	0.47
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.49	0.47
1:A:31:LEU:HD11	9:A:2552:PEG:H31	1.97	0.47
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.50	0.46
1:A:247:GLU:OE1	1:A:250:ARG:NH1	2.49	0.44
1:A:132:GLY:HA3	1:A:143:LEU:HD12	2.00	0.44
1:A:186:PHE:HB3	9:A:2550:PEG:H42	1.99	0.43
1:A:133:LYS:HE2	1:A:134:TYR:CZ	2.53	0.43
1:A:197:PHE:HB2	1:A:223:ILE:HB	2.00	0.42
1:A:366:LEU:HD23	1:A:535:THR:HG21	2.02	0.42
8:A:2543:PGE:H3	10:A:1605:HOH:O	2.18	0.42
1:A:110:THR:OG1	1:A:478[A]:LYS:HG2	2.20	0.41
1:A:282:LEU:O	6:A:2541:MES:H71	2.20	0.41
1:A:355:GLY:HA3	1:A:391:LEU:HD11	2.03	0.41
1:A:330:PHE:CE2	9:A:2549:PEG:H31	2.56	0.41
1:A:515:ARG:HB3	1:A:518:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	539/537 (100%)	510 (95%)	29 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	474/469 (101%)	460 (97%)	14 (3%)	41 53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	129	VAL
1	A	197	PHE
1	A	238	VAL
1	A	288	PHE
1	A	330	PHE
1	A	343	SER
1	A	408	VAL
1	A	430	LEU
1	A	473	TRP
1	A	487	SER
1	A	489	GLU
1	A	490	SER
1	A	499	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	257	ASN
1	A	374	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	B	1	2,1	14,14,15	0.57	0	17,19,21	1.51	2 (11%)
2	NAG	B	2	2	14,14,15	0.56	0	17,19,21	1.00	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	4.30	118.01	112.19
2	B	1	NAG	C6-C5-C4	-2.37	107.46	113.00
2	B	2	NAG	C4-C3-C2	2.19	114.23	111.02

There are no chirality outliers.

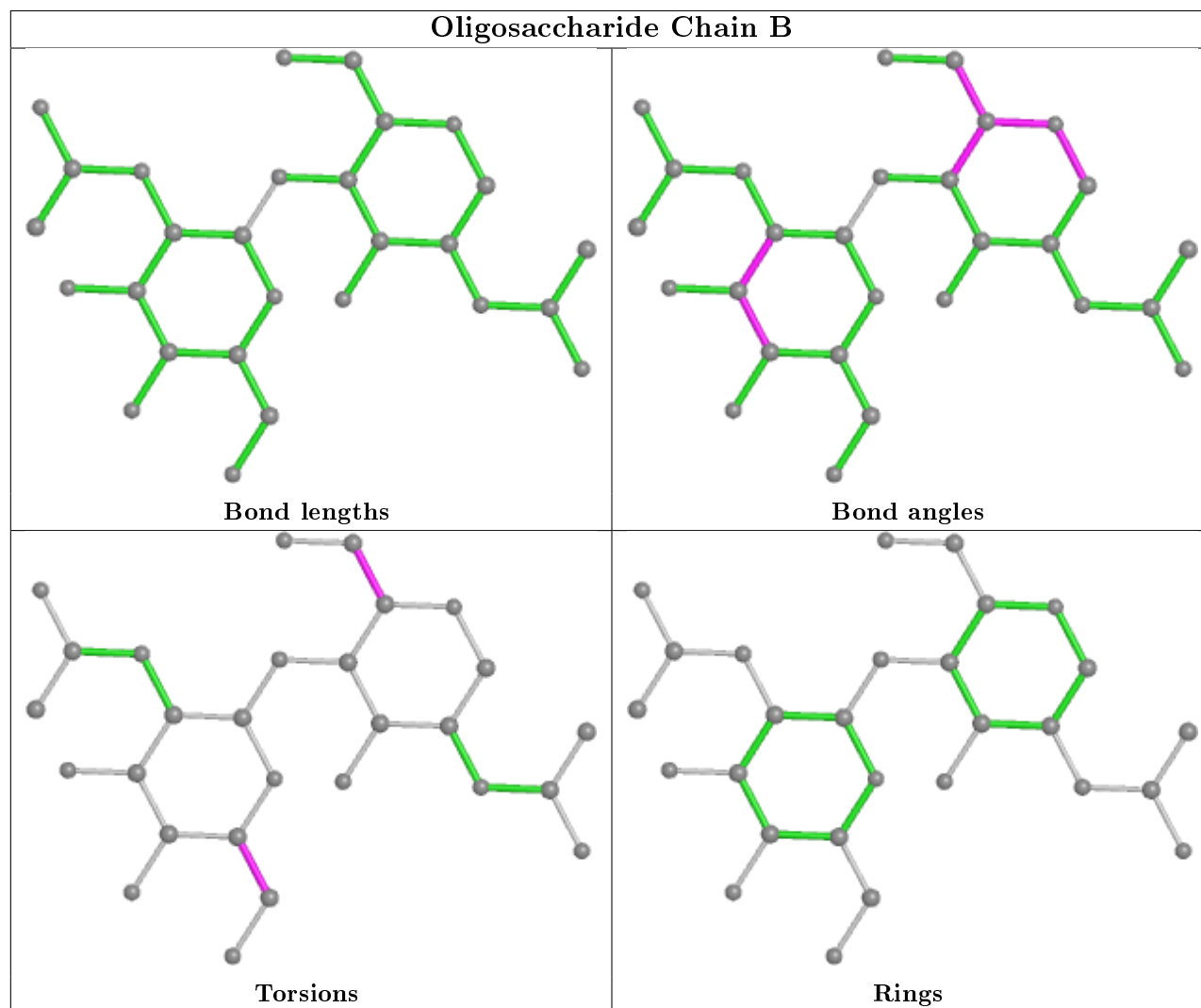
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PG4	A	2542	-	12,12,12	0.95	0	11,11,11	0.82	0
6	MES	A	2541	-	12,12,12	1.59	3 (25%)	14,16,16	1.85	4 (28%)
8	PGE	A	2544	-	9,9,9	0.65	0	8,8,8	0.44	0
9	PEG	A	2550	-	6,6,6	0.80	0	5,5,5	0.50	0
9	PEG	A	2556	-	6,6,6	0.52	0	5,5,5	0.71	0
9	PEG	A	2549	-	6,6,6	0.68	0	5,5,5	0.74	0
8	PGE	A	2543	-	9,9,9	0.65	0	8,8,8	0.48	0
5	GB	A	2540	1	0,3,4	0.00	-	0,3,6	0.00	-
9	PEG	A	2547	-	6,6,6	0.89	0	5,5,5	0.66	0
9	PEG	A	2551	-	6,6,6	1.19	0	5,5,5	1.21	1 (20%)
9	PEG	A	2553	-	6,6,6	0.61	0	5,5,5	0.54	0
3	NAG	A	2538	1	14,14,15	0.59	0	17,19,21	2.59	9 (52%)
8	PGE	A	2545	-	9,9,9	0.81	0	8,8,8	0.49	0
3	NAG	A	2536	1	14,14,15	0.60	0	17,19,21	1.67	6 (35%)
9	PEG	A	2552	-	6,6,6	0.61	0	5,5,5	0.57	0
9	PEG	A	2548	-	6,6,6	0.69	0	5,5,5	0.42	0
8	PGE	A	2546	-	9,9,9	0.64	0	8,8,8	0.39	0
9	PEG	A	2554	-	6,6,6	0.64	0	5,5,5	0.57	0
9	PEG	A	2555	-	6,6,6	0.58	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	A	2545	-	-	3/7/7/7	-
9	PEG	A	2549	-	-	3/4/4/4	-
9	PEG	A	2556	-	-	2/4/4/4	-
8	PGE	A	2546	-	-	2/7/7/7	-
7	PG4	A	2542	-	-	6/10/10/10	-
9	PEG	A	2554	-	-	2/4/4/4	-
6	MES	A	2541	-	-	4/6/14/14	0/1/1/1
8	PGE	A	2543	-	-	3/7/7/7	-
3	NAG	A	2538	1	-	5/6/23/26	0/1/1/1
9	PEG	A	2547	-	-	3/4/4/4	-
9	PEG	A	2555	-	-	2/4/4/4	-
9	PEG	A	2551	-	-	2/4/4/4	-
8	PGE	A	2544	-	-	4/7/7/7	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEG	A	2553	-	-	2/4/4/4	-
3	NAG	A	2536	1	-	2/6/23/26	0/1/1/1
9	PEG	A	2552	-	-	4/4/4/4	-
9	PEG	A	2550	-	-	2/4/4/4	-
9	PEG	A	2548	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2541	MES	C8-S	4.42	1.83	1.77
6	A	2541	MES	O1S-S	2.12	1.51	1.45
6	A	2541	MES	O2S-S	2.08	1.51	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2538	NAG	C2-N2-C7	5.66	130.96	122.90
3	A	2538	NAG	C1-O5-C5	4.61	118.44	112.19
3	A	2538	NAG	C8-C7-N2	4.16	123.14	116.10
6	A	2541	MES	O1-C2-C3	-3.60	103.87	111.80
3	A	2538	NAG	C1-C2-N2	3.35	116.21	110.49
6	A	2541	MES	O3S-S-C8	3.23	111.00	105.77
6	A	2541	MES	C5-N4-C3	3.03	115.66	108.83
3	A	2536	NAG	O5-C1-C2	2.69	115.53	111.29
3	A	2536	NAG	O5-C5-C6	2.63	111.33	107.20
3	A	2538	NAG	O4-C4-C5	2.42	115.31	109.30
3	A	2536	NAG	C1-C2-N2	-2.38	106.42	110.49
3	A	2538	NAG	C4-C3-C2	-2.34	107.58	111.02
9	A	2551	PEG	O2-C3-C4	2.26	120.02	110.07
6	A	2541	MES	C6-C5-N4	-2.25	106.70	110.10
3	A	2538	NAG	O5-C1-C2	-2.21	107.79	111.29
3	A	2536	NAG	C2-N2-C7	2.20	126.04	122.90
3	A	2538	NAG	O5-C5-C6	2.20	110.65	107.20
3	A	2536	NAG	C8-C7-N2	2.12	119.69	116.10
3	A	2538	NAG	O7-C7-N2	-2.10	118.10	121.95
3	A	2536	NAG	C4-C3-C2	2.04	114.00	111.02

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2541	MES	C7-C8-S-O2S
9	A	2548	PEG	O2-C3-C4-O4
9	A	2554	PEG	C4-C3-O2-C2
7	A	2542	PG4	O2-C3-C4-O3
8	A	2546	PGE	O2-C3-C4-O3
3	A	2536	NAG	C8-C7-N2-C2
3	A	2536	NAG	O7-C7-N2-C2
3	A	2538	NAG	C8-C7-N2-C2
3	A	2538	NAG	O7-C7-N2-C2
7	A	2542	PG4	O3-C5-C6-O4
9	A	2550	PEG	O2-C3-C4-O4
6	A	2541	MES	C7-C8-S-O3S
7	A	2542	PG4	O4-C7-C8-O5
9	A	2552	PEG	O2-C3-C4-O4
9	A	2547	PEG	O1-C1-C2-O2
3	A	2538	NAG	C4-C5-C6-O6
8	A	2544	PGE	O1-C1-C2-O2
8	A	2544	PGE	O3-C5-C6-O4
9	A	2549	PEG	O1-C1-C2-O2
9	A	2549	PEG	O2-C3-C4-O4
9	A	2550	PEG	O1-C1-C2-O2
9	A	2553	PEG	O2-C3-C4-O4
8	A	2543	PGE	O2-C3-C4-O3
9	A	2555	PEG	O2-C3-C4-O4
9	A	2556	PEG	O1-C1-C2-O2
8	A	2546	PGE	C3-C4-O3-C5
9	A	2553	PEG	C4-C3-O2-C2
9	A	2549	PEG	C4-C3-O2-C2
8	A	2543	PGE	C6-C5-O3-C4
8	A	2544	PGE	C3-C4-O3-C5
9	A	2551	PEG	C4-C3-O2-C2
9	A	2556	PEG	C4-C3-O2-C2
7	A	2542	PG4	O1-C1-C2-O2
9	A	2548	PEG	O1-C1-C2-O2
9	A	2552	PEG	C4-C3-O2-C2
9	A	2548	PEG	C4-C3-O2-C2
8	A	2543	PGE	C1-C2-O2-C3
6	A	2541	MES	C7-C8-S-O1S
9	A	2554	PEG	O1-C1-C2-O2
8	A	2545	PGE	C6-C5-O3-C4
9	A	2547	PEG	C4-C3-O2-C2
9	A	2552	PEG	O1-C1-C2-O2
3	A	2538	NAG	C3-C2-N2-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	A	2555	PEG	O1-C1-C2-O2
7	A	2542	PG4	C5-C6-O4-C7
8	A	2545	PGE	O1-C1-C2-O2
6	A	2541	MES	C8-C7-N4-C3
3	A	2538	NAG	O5-C5-C6-O6
8	A	2544	PGE	C4-C3-O2-C2
9	A	2547	PEG	C1-C2-O2-C3
8	A	2545	PGE	O2-C3-C4-O3
9	A	2552	PEG	C1-C2-O2-C3
9	A	2548	PEG	C1-C2-O2-C3
7	A	2542	PG4	C1-C2-O2-C3
9	A	2551	PEG	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2541	MES	1	0
8	A	2544	PGE	1	0
9	A	2550	PEG	2	0
9	A	2549	PEG	2	0
8	A	2543	PGE	1	0
9	A	2551	PEG	4	0
9	A	2552	PEG	1	0
9	A	2548	PEG	1	0
9	A	2555	PEG	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	532/537 (99%)	-0.59	5 (0%) 84 83	11, 21, 35, 55	6 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	4.2
1	A	488	GLN	3.5
1	A	485	PRO	3.1
1	A	535	THR	2.1
1	A	257	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

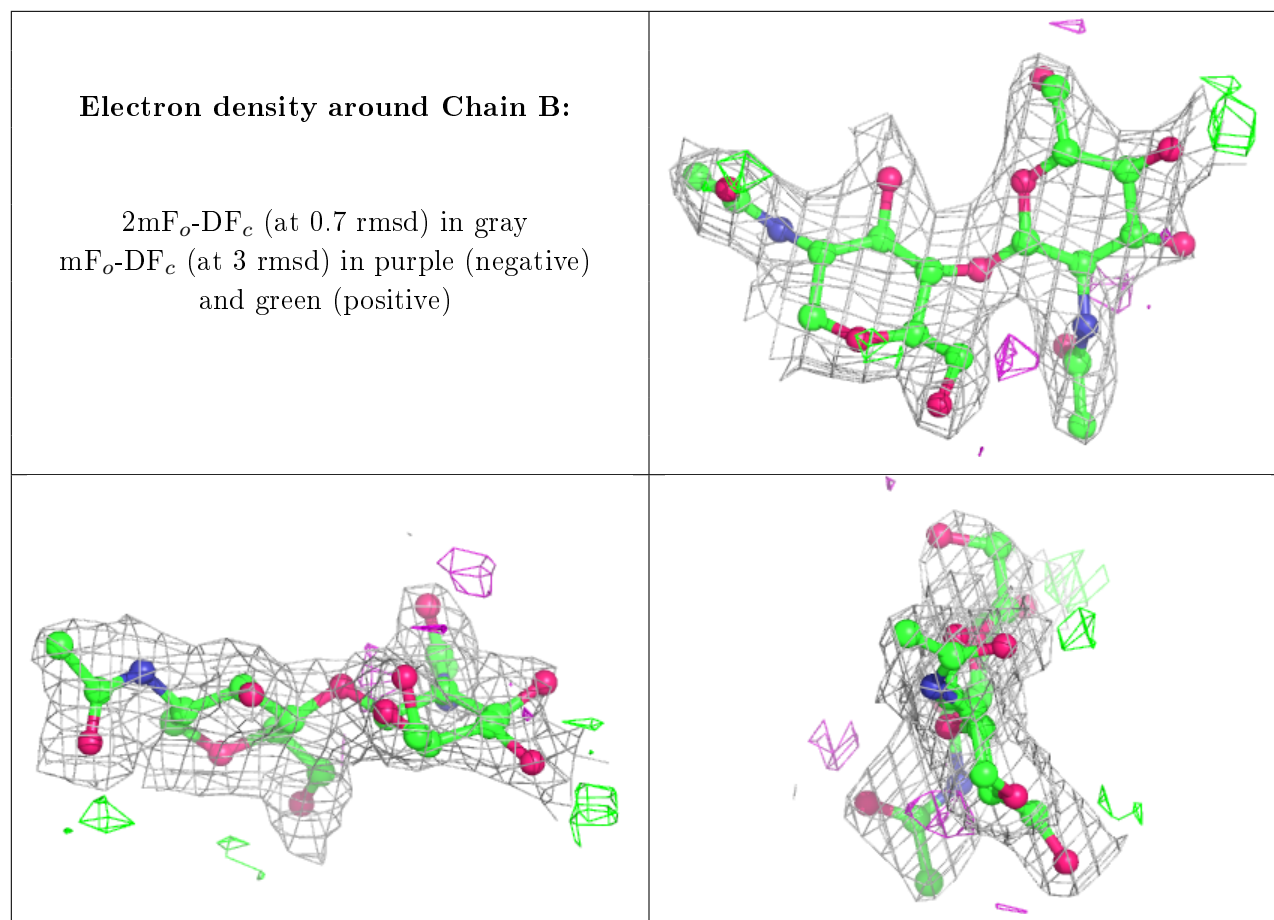
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.81	0.30	55,57,60,60	0
2	NAG	B	1	14/15	0.93	0.15	36,40,45,51	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	PGE	A	2545	10/10	0.69	0.32	62,68,70,71	0
3	NAG	A	2536	14/15	0.71	0.41	65,71,73,73	0
9	PEG	A	2553	7/7	0.76	0.18	60,61,62,63	0
9	PEG	A	2547	7/7	0.80	0.33	47,50,54,54	0
3	NAG	A	2538	14/15	0.82	0.27	49,55,58,58	0
9	PEG	A	2548	7/7	0.83	0.27	59,59,61,62	0
8	PGE	A	2544	10/10	0.83	0.16	48,55,59,59	0
9	PEG	A	2555	7/7	0.83	0.25	54,57,64,65	0
9	PEG	A	2554	7/7	0.86	0.29	60,61,63,64	0
9	PEG	A	2550	7/7	0.87	0.23	48,50,51,51	0
6	MES	A	2541	12/12	0.87	0.18	42,46,52,54	0
7	PG4	A	2542	13/13	0.87	0.33	42,45,48,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	PEG	A	2549	7/7	0.87	0.34	40,41,46,46	0
9	PEG	A	2552	7/7	0.88	0.15	48,52,58,60	0
8	PGE	A	2543	10/10	0.89	0.21	49,51,56,58	0
8	PGE	A	2546	10/10	0.90	0.17	62,65,72,72	0
9	PEG	A	2551	7/7	0.92	0.17	32,34,36,37	0
9	PEG	A	2556	7/7	0.93	0.14	41,42,44,44	0
4	CL	A	2539	1/1	0.95	0.08	53,53,53,53	0
5	GB	A	2540	4/5	1.00	0.12	19,19,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.